Algorithm for NO_2 profile from limb scattering

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Introduction

This document contains a description of the algorithm used for retrieving profiles of nitrogen dioxide (NO_2) from SCIAMACHY limb scattering. It also cites many references which contain addition detail. A similar algorithm was developed in 2001 for OSIRIS and has been maturing [e.g. Sioris *et al.*, 2007].

Forward model

The radiative transfer model (RTM) used and viewing geometry conventions are described in McLinden *et al.* [2002]. The RTM does multiple scattering calculations using the successive orders of scattering technique and accounts for the variation of the solar zenith angle along the line of sight and the sphericity of the atmosphere in photon transmission. The RTM is run in scalar mode, simulating only the 1st element of the Stokes vector. The temperature dependence of the absorption by nitrogen dioxide (NO_2) and ozone (O_3) is included. Clouds below the field of view are neglected. Aerosols are completely neglected in this algorithm. Five orders of scattering are calculated. The fitting window is 434.7-494.9 nm.

Inversion procedure

The inversion procedure follows Sioris *et al.* [2004] and references therein. In short, the retrieval is direct (no *a priori* NO_2 profile knowledge is required) and tried to match measured SCDs to simulated. SCDs SCDs are determined from the measured and simulated radiances using an I_0 (reference spectrum) near TH=50 km. The retrieval range is 11-41 km. Chahine's method is used for the first iteration. Subsequent guesses rely on linear extrapolation or interpolation using the local Jacobian, $dSCD_{TH}/dx_{z=TH}$, where SCD is the NO_2 slant column density at a tangent height (TH) and x is the NO_2 number density at the tangent altitude.

Auxiliary data

Currently, the algorithm does not automatically calculate the TH offset or find cloud top height. These are found first with separate algorithms and stored values of TH offsets and cloud top height serve as input into the NO_2 profile retrieval. The TH determination algorithm is described in Sioris *et al.* [2006] and references therein. Clouds are determined using pixel 312 of channel 6 (~1.23 μm). Starting from the 11th elevation step and proceeding downward, the mean and the standard deviation (σ) of the slope of the natural logarithm of the limb radiance as a function of tangent height are determined for tangent heights between the current elevation step and 15th elevation step. Cloud top height is defined as the highest tangent height for which the local slope departs from the mean slope by more than the empirically-derived threshold of 1.84σ.

All other auxiliary data comes from the RTM's extensive database of surface spectral reflectance values [Koelemeijer *et al.*, 2003] and atmospheres [see McLinden *et al.*, 2002].

Sensitivity and error analysis

Retrieval errors can arise from errors in the forward model or its inputs. Many of the inputs are geophysical (such as surface albedo, temperature profile, etc.). The error due to using only five orders of scattering is <1%. The use of the scalar approximation to model the radiation field also leads to <1% error throughout the stratosphere.

A major source of systematic error comes from pointing. Using the ~305 nm knee, pointing accuracy is expected to be of the order of 300 m. This leads to errors of up to ~10% [Haley *et al.*, 2004] with the bias changing sign between the top and bottom of the retrieved profile. The errors are expected to be smaller than this in the middle of the profile.

At large solar zenith angles (SZAs), the photochemical variation of NO_2 along the line-of-sight and in the incoming solar radiation must be included in the RTM simulations to avoid large errors. The error from neglecting the diurnal variation along the line-of-sight and in the incoming solar beam for SZA<85° is <40% and is <25% above 20 km [McLinden *et al.*, accepted].

The initial guess sensitivity is <4% at altitudes below 35 km, even for SZA=89° [Sioris *et al.*, 2003] and is 2.3% at 19 km for SZA=57°, and decreases monotonically above that. For even smaller SZAs, the sensitivity to the initial guess is expected to be higher than 2.3%, but has not been quantified.

The neglect of clouds below the field of view also leads to significant errors in high sun conditions. For SZA=30°, the error reaches 22% in the upper stratosphere (37 km) and 11% in the lower stratosphere (19 km). At SZA=57°, the error is 9% and 7% in the upper and lower stratosphere, respectively and becomes a minor error source for near-grazing solar elevation angles [Sioris *et al.*, 2003].

The impact of errors in the assumed stratospheric aerosol concentration is <5% even for a change from background conditions to a "moderate volcanic" profile [Sioris *et al.*, 2003]. The retrieval also shows a weak sensitivity to expected errors in pressure and temperature.

Other error sources have not been considered yet.

<u>Algorithm validation</u>

A coincidence with HALOE [Sioris *et al.*, 2004] showed typical agreement of 8% between 17 and 41 km, after diurnal scaling with a photochemical model to match local times. The reader is referred to Butz *et al.* [2006] for further validation results versus the DOAS balloon-borne instrument. This study shows that profiles retrieved with this algorithm may have residual pointing errors.

<u>Recommendations for product validation</u>

Profile measurements in the Antarctic vortex are recommended. Validation measurements are also needed after thunderstorms to see if large increases in NO_2 detected by in-situ instruments are observed by SCIAMACHY. Our current results show much lower concentrations of NO_2 in the upper troposphere than unpublished in-situ data from a recent summertime campaign (INTEX-NA), but this may result from a clear sky bias that we have due to the fact that SCIAMACHY profile retrieval only extends down to cloud tops. Note that in-situ instruments can measure below cloud top.

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